Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Explicit consideration of surface structures for work function calculations SEUNGCHUL KIM, ANDREW M. RAPPE, Department of Chemistry, University of Pennsylvania — We investigate the effects of atomic structure of surfaces on work functions, using density functional theory (DFT) calculations. Despite the well-known orientation dependence of work functions, the effect of geometric structure of surfaces on work functions is rarely considered. To examine whether the atomic structure of a surface is important to the work function, we perform DFT calculations of thick slabs in the periodic supercell. We then extract the energy levels of the occupied states relative to the vacuum level. Surfaces of oxides, such as $BaTiO_3$ (001), $SrTiO_3$ (001), and TiO_2 (110), are especially well-tested because of their various reconstructed structures. Our calculations show that, even for the same surface orientation, the difference in stoichiometry and geometry of the surface gives rise to substantially different work functions. This finding strongly implies that the atomic structures of surfaces must be explicitly taken into account in predicting work functions of materials.

Seungchul Kim
Department of Chemistry, University of Pennsylvania

Date submitted: 10 Nov 2011 Electronic form version 1.4